Quantum phase transitions in a frustrated orthogonal-dimer $S = 1$ spin system

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Abstract

We investigate quantum phase transitions in a quasi-one dimensional orthogonal-dimer $S = 1$ spin chain by means of the exact diagonalization. By taking into account the effect of the interchain coupling, we discuss how the distinct spin-gap phases found in the orthogonal-dimer chain are adiabatically connected to those in the two-dimensional Shastry-Sutherland model for the compounds $SrCu_2(BO_3)_2$ and Nd_2BaZnO_5.

Key words: orthogonal-dimer structure; exact diagonalization; frustration

Frustrated quantum spin systems have attracted current interest. A typical example is the cuprate $SrCu_2(BO_3)_2$,[1] where the Cu^{2+} ions sit on the orthogonal-dimer structure, [2,3] shown in Fig. 1. In

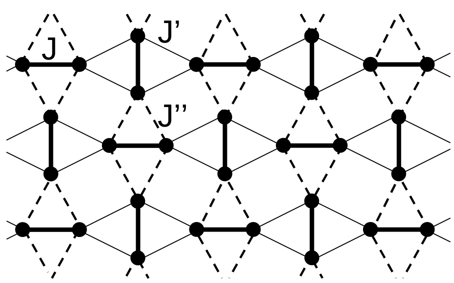

Fig. 1. The orthogonal-dimer structure. The bold, thin and dashed lines represent the exchange couplings J, J' and J'', respectively.

this material, novel magnetic properties were observed such as magnetization plateaus, excited states without dispersion,[1,4] which stimulate further theoretical investigations of the Shastry-Sutherland model.[3,5,6] More recently, a new orthogonal-dimer compound Nd_2BaZnO_5 was synthesized,[7] where the local moment $J = 9/2$ shows an antiferromagnetic order below $T_N = 2.4K$. Therefore, it is desirable to clarify how a higher spin generalization ($S > 1/2$), together with the competing exchange couplings, affects the ground state properties of such frustrated spin systems.

In our previous paper,[8] we have dealt with the orthogonal-dimer spin chain ($J'' = 0$) with an arbitrary spin S and have shown that first-order quantum phase transitions occur ($2S$) times. In particular, in the $S = 1$ system, the Haldane spin-gap phase exists between the dimer and the plaquette phases. It is naively expected that the intermediate phase is not stable against the interchain coupling since such a quasi-one dimensional $S = 1$ spin chain is usually driven to the antiferromagnetic phase.[9–11] In this paper, we deal with the $S = 1$ orthogonal-dimer system by means of the exact diagonalization to discuss how the interchain coupling affects the spin gap phases realized in the chain.

We consider here the model Hamiltonian with the orthogonal-dimer structure as,

$$H = \sum_{(ij)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (1)$$

where $\mathbf{S}_j$ indicates the $S = 1$ spin operator at the jth site, and $J_{ij} = J, J'$ and J'' represent the intra-dimer, the inter-dimer and the interchain couplings, which are

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all assumed to be antiferromagnetic. To clarify how the spin-gap phases in the chain system are adiabatically connected to those in the 2D Shastry-Sutherland model, we perform the exact diagonalization of the orthogonal-dimer $S = 1$ spin system ($N = 4 \times 4$) with periodic boundary condition. The results are shown in Fig. 2. When $J'' = 0$, the system is reduced to the $S = 1$ orthogonal-dimer spin chain, where first-order quantum phase transitions occur among three spin-gap phases. [8] Although the introduction of the interchain

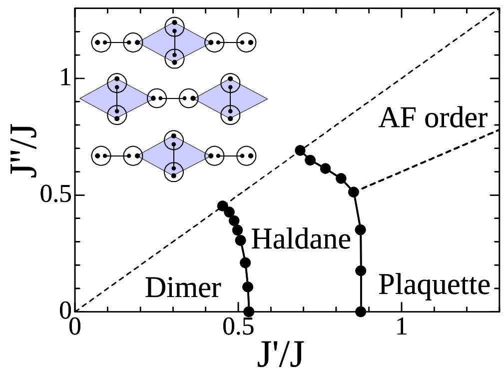

Fig. 2. The phase diagram of the orthogonal-dimer spin $S = 1$ system. The solid lines indicate the phase boundary where the first-order transition occurs. The dashed line indicates the phase boundary between the plaquette and the antiferromagnetically ordered phases, where the second-order transition occurs.

coupling J'' enhances antiferromagnetic correlations, the dimer phase is still stable in the small J' and J'' region since the assembly of dimers shown by the bold line in Fig. 1 is the exact eigenstate of the Hamiltonian. It is remarkable that the frustration-induced Haldane phase in the chain persists even in the 2D Shastry-Sutherland model ($J' = J''$). The nature of the Haldane phase is clearly described by the Valence Bond Solid, [12] where the spin-gap state is represented by the assembly of the singlet bonds between the decomposed $S = 1/2$ spins. In the frustration-induced Haldane phase, one of the decomposed $S = 1/2$ spins at each site is connected to the nearest neighbor spin to form the singlet-dimer on the strong-coupling bond, as shown in the inset of Fig. 2. Another decomposed spin is connected to other three spins to form the plaquette singlet. Therefore, this phase is composed of a periodic arrangement of the dimer and the plaquette singlets discussed in the $S = 1/2$ Shastry-Sutherland model, [5] and is stable against the interchain coupling. In the plaquette phase, the spin gap continuously decreases with increasing the interchain coupling J'', and the system may be driven to the antiferromagnetically ordered phase. Though it is difficult to determine this boundary, we think that the plaquette phase may not persist on the Shastry-Sutherland line ($J' = J''$) since the system with $S = 1$ spins favors the classical Neel ordered state, in contrast to the plaquette phase in the $S = 1/2$ Shastry-Sutherland model.[5,13,14] We show this phase boundary in Fig. 2 as a guide to eyes. Although our calculation is restricted to a small system, we believe that the frustration-induced spin-gap phases discussed here give the correct phase diagram of the $S = 1$ Shastry-Sutherland model.[2]

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